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Study on stationary solutions to the problem of phytoplankton dynamics considering transformation of phosphorus, nitrogen and silicon compounds*

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Исследование стационарных решений задачи динамики фитопланктона с учетом трансформации соединений фосфора, азота и кремния***

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Introduction. The solution to the problem of transformation of phosphorus, nitrogen and silicon forms is studied. This problem arises under modeling phytoplankton dynamics in shallow-water bodies including the Azov Sea. The phytoplankton dynamics model is formulated as a boundary value problem for the system of diffusion-convection-response equations and takes into account the absorption and release of nutrients by phytoplankton, as well as the transition of nutrients from one compound to another. To calculate the initial conditions and parameters of the equations under which the steady-state regime occurs, the software is developed, which is based on the model describing changes in phytoplankton concentrations without considering current effects. This model is represented by a system of inhomogeneous differential equations. Based on the developed software, the initial conditions and parameters of the phytoplankton dynamics model in the Azov Sea are calculated experimentally.

Materials and Methods. A 3D model of phytoplankton dynamics is considered taking into account the transformation of phosphorus, nitrogen and silicon compounds based on the system of nutrient transport equations. The case of a spatially uniform distribution of substances is considered to specify the parameters of the model at which the stationary modes occur. Because of simplification, a system of ordinary differential equations solved through the Runge-Kutta method is obtained.

Research Results. The software is developed to specify the initial conditions and parameters of the phytoplankton dynamics model considering the transformation of phosphorus, nitrogen and silicon compounds.

Several numerical experiments are performed under the assumption that the development of phytoplankton is limited by

Введение. Работа посвящена исследованию решения задачи трансформации форм фосфора, азота и кремния. Данная проблема возникает при моделировании динамики фитопланктона в мелководных водоемах, в том числе в Азовском море. Модель динамики фитопланктона сформулирована как краевая задача для системы уравнений диффузии-конвекции-реакции и учитывает поглощение и выделение питательных веществ фитопланктоном, а также переход питательных веществ из одного соединения в другое. Для расчета начальных условий и параметров уравнений, при которых наступает стационарный режим, разработано программное обеспечение, основой которого послужила модель, описывающая изменения концентраций фитопланктона без учета влияния течений. Данная модель представлена системой неоднородных обыкновенных дифференциальных уравнений. На основе разработанного программного обеспечения экспериментальным образом рассчитаны начальные условия и параметры модели динамики фитопланктона в Азовском море.

Материалы и методы. Рассматривается трехмерная модель динамики фитопланктона с учетом трансформации соединений фосфора, азота и кремния, основанная на системе уравнений транспорта биогенных веществ. Для уточнения параметров модели, при которых наступают стационарные режимы, рассматривается случай пространственно-однородного распределения субстанций. В результате упрощения получена система обыкновенных дифференциальных уравнений, которая решена методом Рунге-Кутты.

Результаты исследования. Разработано программное обеспечение для уточнения начальных условий и параметров модели динамики фитопланктона с учетом трансформации соединений фосфора, азота и кремния. Проведены несколько численных экспериментов в предположении, что развитие фитопланктона лимитируется единственным биогенным веществом. В результате вычисли-

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a single biogenic substance. As a result of the computational experiment, it can be seen that with the obtained values of the initial concentrations and parameters of the equations, stationary modes occur for the system of ordinary differential equations describing the case of the spatially uniform distribution of substances.

Discussion and Conclusions. The mathematical model of the transformation of phosphorus, nitrogen and silicon forms in the problem of phytoplankton dynamics is studied. Stationary modes for the system of ordinary differential equations are obtained, for which the values of the system parameters and initial conditions are determined. The results obtained can be used in further simulation of the phytoplankton dynamics considering the transformation of phosphorus, nitrogen and silicon compounds with account for convection-diffusion, salinity, and temperature.

Keywords: phytoplankton, phosphorus, nitrogen, silicon, biogen, chemical-biological source, convection-diffusion-response equation, Cauchy problem for system of ordinary differential equations, stationary mode.

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Introduction. Because of the development of major cities on the coast of shallow water bodies and river systems that flow into these water bodies, eutrophication has become more frequent. The growth of algae in reservoirs is caused by an increase in the flow of nitrogen and phosphorus compounds from the adjacent land areas. Each water body is unique and requires a thorough study. Field investigations [1] and mathematical modeling are used to explore water bodies. Without downplaying the role of field experiments, we can say that mathematical modeling is less costly, and it allows us to predict the behavior of the ecosystem.

To study the Sea of Azov, a three-dimensional model of hydrodynamics [2, 3] including the equations of motion in three spatial directions was developed. In [4], this model was made for the case of dynamic rebuilding of the computational domain geometry due to the tidal effects. The investigation of this model accuracy is given in [5]. In [6–8], the reconstruction of an ecological catastrophe that occurred in 2001 caused by an excessive concentration of algae in the eastern part of the Sea of Azov is given. In [9], methods of controlling the suffocation phenomena arising in the Sea of Azov were proposed. The [10–12] papers are devoted to studying the dynamics of phyto- and zooplankton.

The water condition in shallow water bodies is changing rapidly, and mathematical models need to be refined. The parameters determination of the three-dimensional model of the phyto- and zooplankton dynamics is laborious; therefore, it is proposed to use a simplified model to calculate these parameters.

The work objective is to improve the parameters of the model of the phytoplankton dynamics considering the transformation of phosphorus, nitrogen and silicon compounds, under which stationary regimes occur with the assumption of a spatially uniform distribution of substances.

Materials and Methods. The model is based on the system of equations for the transport of nutrients [15, 16], the form of which for each F_i model block is

тельного эксперимента видно, что при полученных значениях начальных концентраций и параметров уравнений наступают стационарные режимы для системы обыкновенных дифференциальных уравнений, описывающей случай пространственно-равномерного распределения субстанций.

Обсуждение и заключения. В работе исследована математическая модель трансформации форм фосфора, азота и кремния в задаче динамики фитопланктона.

Получены стационарные режимы для системы обыкновенных дифференциальных уравнений, для которых определены значения параметров системы и начальные условия. Полученные результаты могут быть использованы в процессе дальнейшего моделирования динамики фитопланктона с учетом трансформации соединений фосфора, азота и кремния с учетом конвекции-диффузии, солёности, температуры.

Ключевые слова: фитопланктон, фосфор, азот, кремний, биоген, химико-биологический источник, уравнение конвекции-диффузии-реакции, задача Коши для системы обыкновенных дифференциальных уравнений, стационарный режим.

Образец для цитирования. Белова, Ю. В. Исследование стационарных решений задачи динамики фитопланктона с учетом трансформации соединений фосфора, азота и кремния / Ю. В. Белова [и др.] // Вестник Донского гос. техн. ун-та. — 2019. — Т.19, №1. — С. 4–12. <https://doi.org/10.23947/1992-5980-2019-19-1-4-12>

$$\frac{\partial q_i}{\partial t} + u \frac{\partial q_i}{\partial x} + v \frac{\partial q_i}{\partial y} + w \frac{\partial q_i}{\partial z} = \text{div}(k \text{ grad } q_i) + R_{q_i}, \quad (1)$$

where q_i is concentration of the i -th component, [mg/l]; $i \in M$, $M = \{F_1, F_2, F_3, PO_4, POP, DOP, NO_3, NO_2, NH_4, Si\}$; $\{u, v, w\}$ are components of the velocity vector of the water flow, [m/s]; k is turbulent exchange coefficient, [m²/s]; R_{q_i} is function-source of nutrients, [mg/l · s].

In equation (1), i index indicates the type of substance (Table 1).

Table 1

Biogenic substances in model of phytoplankton dynamics

No.	Notation	Name
1	F ₁	Chlorella vulgaris green algae
2	F ₂	Aphanizomenon flos-aquae green-blue algae
3	F ₃	Skeletonema costatum diatom
4	PO ₄	phosphates
5	POP	suspended organic phosphor
6	DOP	soluble organic phosphor
7	NO ₃	nitrates
8	NO ₂	nitrites
9	NH ₄	ammonium
10	Si	soluble inorganic silica (silicic acids)

Chemical and biological reactions are described by the following equations $R_{F_i} = C_{F_i} (1 - K_{F_iR}) q_{F_i} - K_{F_iD} q_{F_i} - K_{F_iE} q_{F_i}$,

$$i = 1, 3,$$

$$R_{POP} = \sum_{i=1}^3 s_P K_{F_iD} q_{F_i} - K_{PD} q_{POP} - K_{PN} q_{POP},$$

$$R_{DOP} = \sum_{i=1}^3 s_P K_{F_iE} q_{F_i} + K_{PD} q_{POP} - K_{DN} q_{DOP},$$

$$R_{PO_4} = \sum_{i=1}^3 s_P C_{F_i} (K_{F_iR} - 1) q_{F_i} + K_{PN} q_{POP} + K_{DN} q_{DOP},$$

$$R_{NH_4} = \sum_{i=1}^3 s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(2)}(q_{NH_4})}{f_N(q_{NO_3}, q_{NO_2}, q_{NH_4})} q_{F_i} + \sum_{i=1}^3 s_N (K_{F_iD} + K_{F_iE}) q_{F_i} - K_{42} q_{NH_4},$$

$$R_{NO_2} = \sum_{i=1}^3 s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(1)}(q_{NO_3}, q_{NO_2}, q_{NH_4})}{f_N(q_{NO_3}, q_{NO_2}, q_{NH_4})} \cdot \frac{q_{NO_2}}{q_{NO_2} + q_{NO_3}} q_{F_i} + K_{42} q_{NH_4} - K_{23} q_{NO_2},$$

$$R_{NO_3} = \sum_{i=1}^3 s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(1)}(q_{NO_3}, q_{NO_2}, q_{NH_4})}{f_N(q_{NO_3}, q_{NO_2}, q_{NH_4})} \cdot \frac{q_{NO_3}}{q_{NO_2} + q_{NO_3}} q_{F_i} + K_{23} q_{NO_2},$$

$$R_{Si} = s_{Si} C_{F_3} (K_{F_3R} - 1) q_{F_3} + s_{Si} K_{F_3D} q_{F_3}.$$

Here, K_{F_iR} is specific breathing rate of phytoplankton; K_{F_iD} is specific die-off rate of phytoplankton; K_{F_iE} is specific excretion rate of phytoplankton; K_{PD} is specific rate of POP autolysis; K_{PN} is coefficient of POP phosphatification; K_{DN} is coefficient of DOP phosphatification; K_{42} is specific rate of ammonium oxidation to nitrites under nitrification; K_{23} is specific rate of nitrite oxidation to nitrates under nitrification; s_P , s_N , s_{Si} are normalization coefficients between the content of N, P, Si in organic matter.

Phytoplankton growth rate is determined by the following expressions:

$$C_{F_{1,2}} = K_{NF_{1,2}} \min \{ f_P(q_{PO_4}), f_N(q_{NO_3}, q_{NO_2}, q_{NH_4}) \},$$

$$C_{F_3} = K_{NF_3} \min \{ f_P(q_{PO_4}), f_N(q_{NO_3}, q_{NO_2}, q_{NH_4}), f_{Si}(q_{Si}) \},$$

where K_{NF} is maximum specific phytoplankton growth rate.

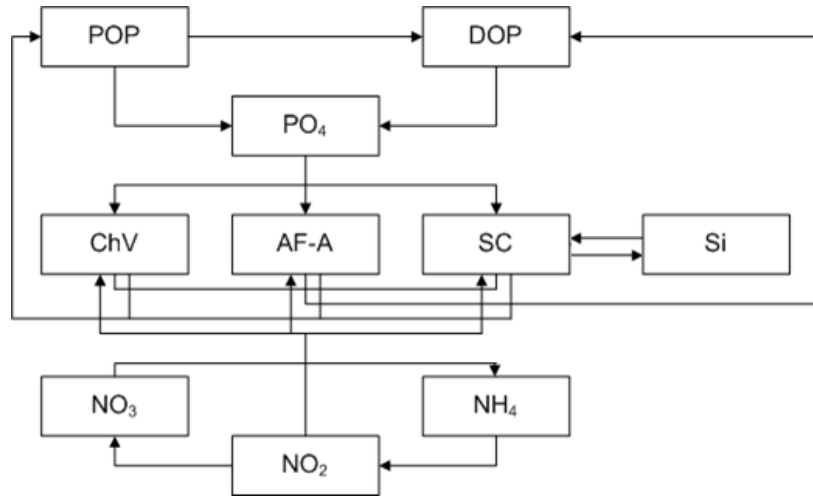


Fig. 1. Model scheme of biogeochemical transformation of phosphorus, nitrogen and silica forms

Functions describing nutrient content

– for phosphorus: $f_P(q_{PO_4}) = \frac{q_{PO_4}}{q_{PO_4} + K_{PO_4}}$,

where K_{PO_4} is phosphates half saturation constant;

– for silica: $f_{Si}(q_{Si}) = \frac{q_{Si}}{q_{Si} + K_{Si}}$,

where K_{Si} is silica half saturation constant;

– for nitrogen: $f_N(q_{NO_3}, q_{NO_2}, q_{NH_4}) = f_N^{(1)}(q_{NO_3}, q_{NO_2}, q_{NH_4}) + f_N^{(2)}(q_{NH_4})$,

$$f_N^{(1)}(q_{NO_3}, q_{NO_2}, q_{NH_4}) = \frac{(q_{NO_3} + q_{NO_2}) \exp(-K_{psi} q_{NH_4})}{K_{NO_3} + (q_{NO_3} + q_{NO_2})}, \quad f_N^{(2)}(q_{NH_4}) = \frac{q_{NH_4}}{K_{NH_4} + q_{NH_4}},$$

where K_{NO_3} is nitrates half saturation constant, K_{NH_4} is ammonium half saturation constant, K_{psi} is ammonium inhibition ratio.

For the system (1), it is necessary to specify the vector field of the water flow velocities, as well as q_i initial values of the concentration functions

$$q_i(x, y, z, 0) = q_i^0(x, y, z), \quad (x, y, z) \in \bar{G}, \quad t = 0, \quad i \in M. \quad (2)$$

Assume Σ boundary of G cylindrical region is piecewise smooth and $\Sigma = \Sigma_H \cup \Sigma_o \cup \sigma$, where Σ_H is surface of the reservoir bottom, Σ_o is still water surface, σ is lateral (cylindrical) surface. Suppose u_n is vector component of the water flow velocity normal to Σ , and n is outward normal vector to Σ . For q_i concentrations, we assume:

– on side boundary:

$$q_i = 0, \quad \text{on } \sigma, \quad \text{if } u_n < 0, \quad i \in M; \quad (3)$$

$$\frac{\partial q_i}{\partial n} = 0, \quad \frac{\partial q_i}{\partial n} = 0, \quad \text{on } \sigma, \quad \text{if } u_n \geq 0, \quad i \in M;$$

– on Σ_o there is reservoir surface:

$$\frac{\partial q_i}{\partial z} = 0, \quad i \in M; \quad (5)$$

– on the bottom Σ_H :

$$k \frac{\partial q_i}{\partial z} = \varepsilon_{1,i} q_i, \quad i \in \{F_1, F_2, F_3\},$$

$$k \frac{\partial q_i}{\partial z} = \varepsilon_{2,i} q_i, \quad i \in \{\text{PO}_4, \text{POP}, \text{DOP}, \text{NO}_3, \text{NO}_2, \text{NH}_4, \text{Si}\}, \quad (6)$$

where $\varepsilon_{1,i}$, $\varepsilon_{2,i}$ are sedimentation rates of algae and nutrients to the bottom.

Stationary Mode. Consider the case of a spatially uniform distribution of substances (phytoplankton, forms of phosphorus, nitrogen and silica); then each of the equations (1) is simplified; and as a result, we get the following system of ordinary differential equations (ODE):

$$\begin{aligned} \frac{dq_{F_i}}{dt} &= C_{F_i} (1 - K_{F_iR}) q_{F_i} - K_{F_iD} q_{F_i} - K_{F_iE} q_{F_i}, \quad i = \overline{1,3}, \\ \frac{dq_{\text{POP}}}{dt} &= \sum_{i=1}^3 s_P K_{F_iD} q_{F_i} - K_{PD} q_{\text{POP}} - K_{PN} q_{\text{POP}}, \\ \frac{dq_{\text{DOP}}}{dt} &= \sum_{i=1}^3 s_P K_{F_iE} q_{F_i} + K_{PD} q_{\text{POP}} - K_{DN} q_{\text{DOP}}, \\ \frac{dq_{\text{PO}_4}}{dt} &= \sum_{i=1}^3 s_P C_{F_i} (K_{F_iR} - 1) q_{F_i} + K_{PN} q_{\text{POP}} + K_{DN} q_{\text{DOP}}, \\ \frac{dq_{\text{NH}_4}}{dt} &= \sum_{i=1}^3 s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(2)}(\text{NH}_4)}{f_N(\text{NO}_3, \text{NO}_2, \text{NH}_4)} q_{F_i} + \sum_{i=1}^3 s_N (K_{F_iD} + K_{F_iE}) q_{F_i} - K_{42} q_{\text{NH}_4}, \\ \frac{dq_{\text{NO}_2}}{dt} &= \sum_{i=1}^3 s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(1)}(\text{NO}_3, \text{NO}_2, \text{NH}_4)}{f_N(\text{NO}_3, \text{NO}_2, \text{NH}_4)} \cdot \frac{q_{\text{NO}_2}}{q_{\text{NO}_2} + q_{\text{NO}_3}} q_{F_i} + K_{42} q_{\text{NH}_4} - K_{23} q_{\text{NO}_2}, \\ \frac{dq_{\text{NO}_3}}{dt} &= \sum_{i=1}^3 s_N C_{F_i} (K_{F_iR} - 1) \frac{f_N^{(1)}(\text{NO}_3, \text{NO}_2, \text{NH}_4)}{f_N(\text{NO}_3, \text{NO}_2, \text{NH}_4)} \cdot \frac{q_{\text{NO}_3}}{q_{\text{NO}_2} + q_{\text{NO}_3}} q_{F_i} + K_{23} q_{\text{NO}_2}, \\ \frac{dq_{\text{Si}}}{dt} &= s_{\text{Si}} C_{F_3} (K_{F_3R} - 1) q_{F_3} + s_{\text{Si}} K_{F_3D} q_{F_3}. \end{aligned} \quad (7)$$

We solve the system of ordinary differential equations by the Runge – Kutta method [15–17]. We will conduct several numerical experiments, assuming that the development of phytoplankton depends on a single limiting substance.

Research Results. For the ODE system (7), we calculate the initial conditions and parameters of the equations at which the stationary regimes occur. Let us take the initial concentration values: $q_{F_1}(0) = 2.5 \text{ mg/l}$, $q_{F_2}(0) = 2.6 \text{ mg/l}$, $q_{F_3}(0) = 0.91 \text{ mg/l}$, $q_{\text{POP}}(0) = 0.07 \text{ mg/l}$, $q_{\text{DOP}}(0) = 0.07 \text{ mg/l}$, $q_{\text{PO}_4}(0) = 0.005 \text{ mg/l}$, $q_{\text{NH}_4}(0) = 0.11 \text{ mg/l}$, $q_{\text{NO}_2}(0) = 0.0178 \text{ mg/l}$, $q_{\text{NO}_3}(0) = 0.304 \text{ mg/l}$, $q_{\text{Si}}(0) = 0.4 \text{ mg/l}$; coefficients: $K_{NF_1} = 2.8 \text{ day}^{-1}$, $K_{F_1R} = 0.15 \text{ day}^{-1}$, $K_{F_1D} = 0.05 \text{ day}^{-1}$, $K_{F_2E} = 0.15 \text{ day}^{-1}$, $K_{PD} = 0.015 \text{ day}^{-1}$, $K_{PN} = 0.02 \text{ day}^{-1}$, $K_{DN} = 0.1 \text{ day}^{-1}$, $K_{42} = 0.9 \text{ day}^{-1}$, $K_{23} = 2.5 \text{ day}^{-1}$, $K_{pSi} = 1.46 \text{ day}^{-1}$, $s_P = 0.01$, $s_N = 0.016$, $s_{\text{Si}} = 0.023$, $K_{\text{PO}_4} = 0.024$, $K_{\text{NO}_3} = 3.0$, $K_{\text{NH}_4} = 2.0$, $K_{\text{Si}} = 3.0$.

The obtained stationary modes of the ODE system (7) on the assumption that the development of phytoplankton is limited by a single nutrient (phosphorus, nitrogen or silica) are shown in Fig. 2–4, respectively. Fig. 2 describes the effect of phosphorus on the development of various phytoplankton species; Fig. 3 describes the effect of nitrogen on the development of various phytoplankton species; Fig. 4 describes the effect of nitrogen on diatom development.

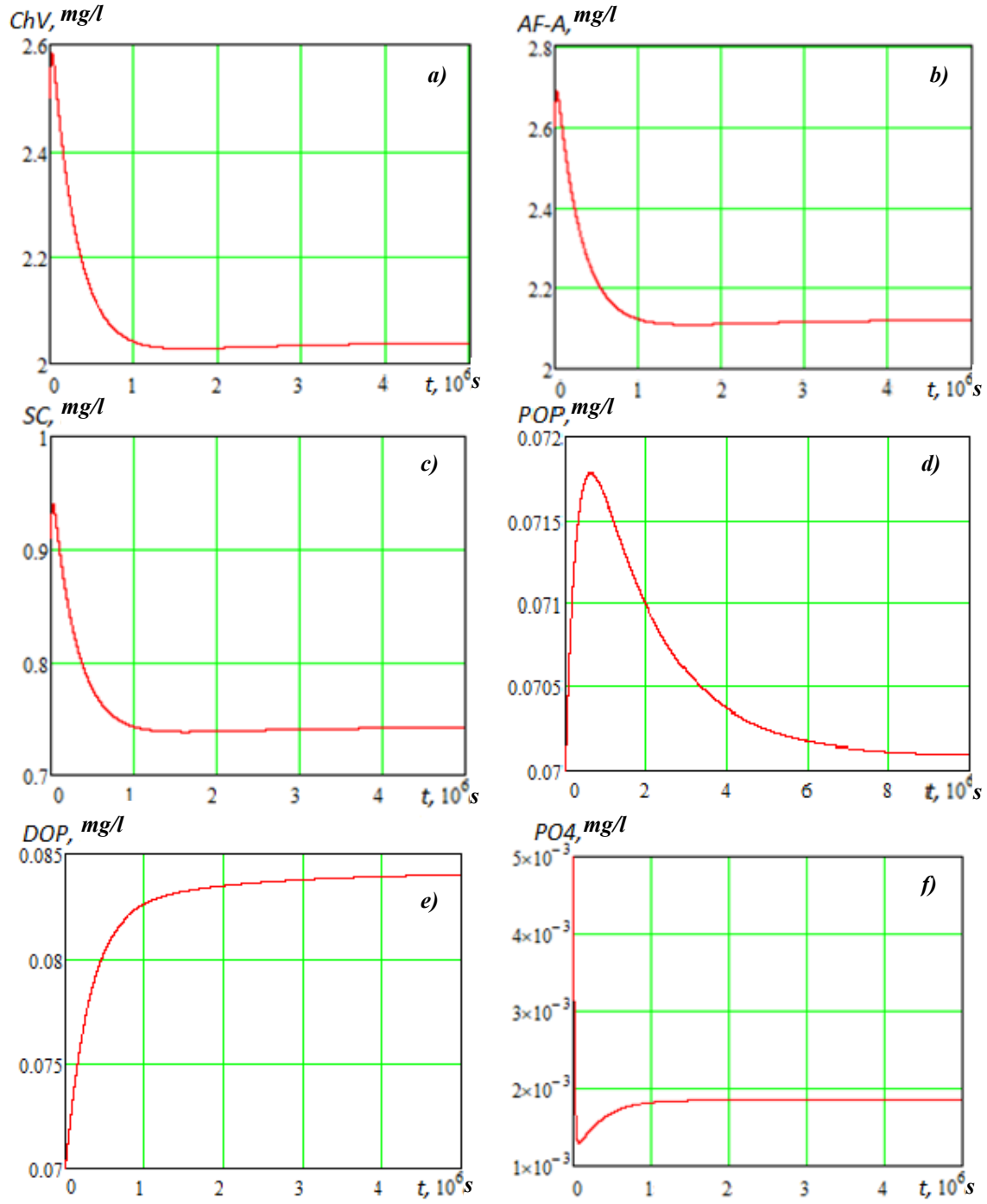


Fig. 2. Stationary mode of ODE system under assumption that phytoplankton development is limited by phosphorus: a) green algae (ChV), b) green-blue algae ($AF-A$), c) diatom (SC), d) suspended organic phosphorus (POP), e) soluble organic phosphorus (DOP), f) phosphates (PO_4)

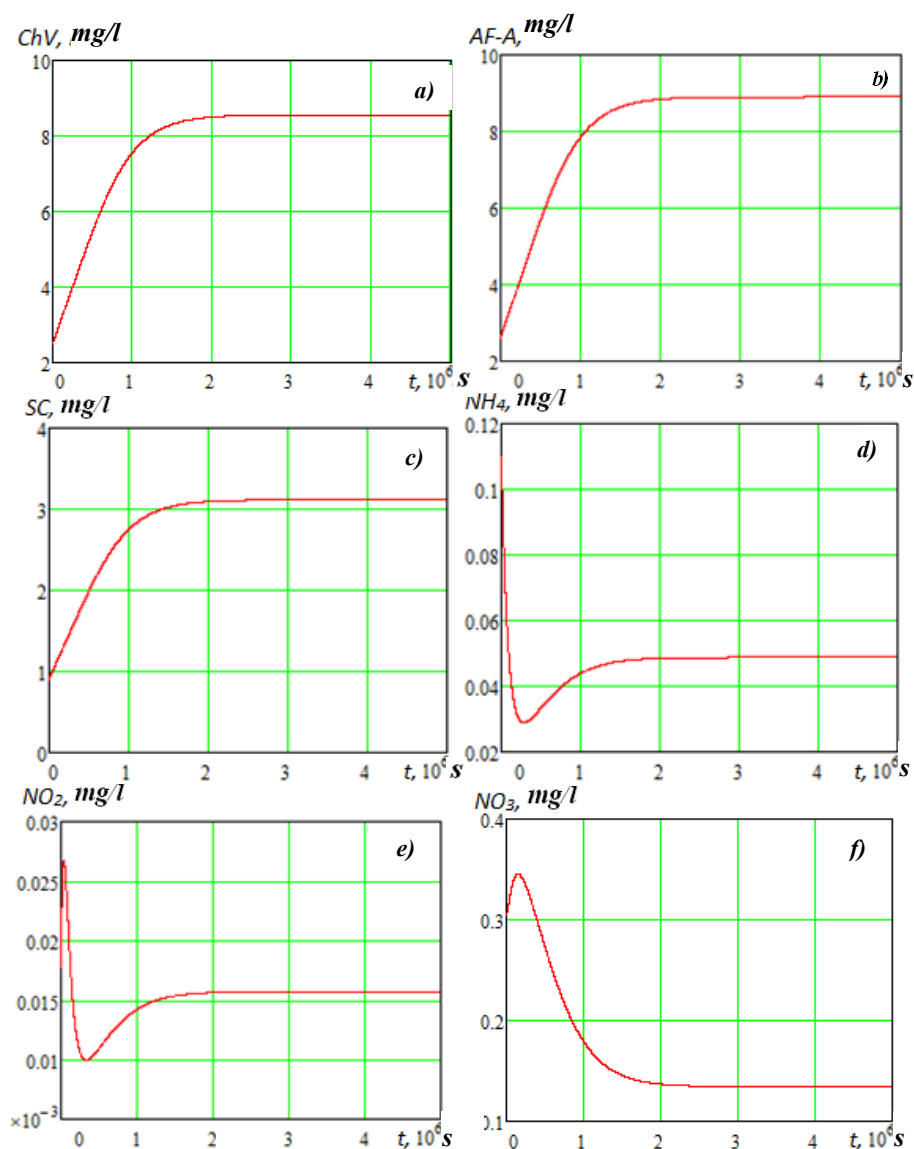


Fig. 3. Stationary mode of ODE system under assumption that phytoplankton development is limited by nitrogen: a) green algae (ChV), b) green-blue algae ($AF-A$), c) diatom (SC), d) ammonium (NH_4), e) nitrites (NO_2), f) nitrates (NO_3).

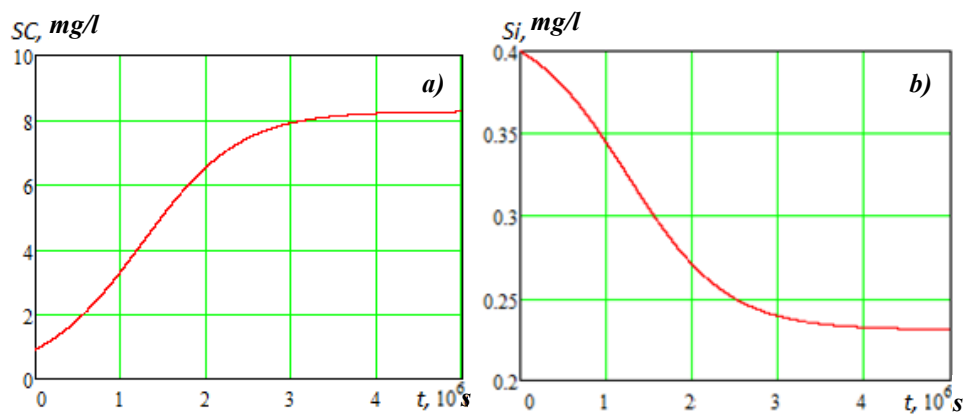


Fig. 4. Stationary mode of ODE system under assumption that phytoplankton (diatoms) development is limited by silica: a) diatom (SC), b) silica (Si).

The result of the computational experiment shows that with the above values of the initial concentrations and parameters of the equations, stationary modes occur for the ODE system (7), which describes the case of a spatially uniform distribution of substances. The obtained values will be used in further simulation of the spatially inhomogeneous distribution of substances, saltness and temperature considering the movement of the aquatic environment [18].

Conclusion. A mathematical model of the transformation of forms of phosphorus, nitrogen and silica in the problem of phytoplankton dynamics is studied in the paper. The case of spatially uniform distribution of substances (phytoplankton, forms of phosphorus, nitrogen and silica) is considered. The system is divided into three systems of ordinary differential equations, each of which simulates the dependence of phytoplankton growth on a single nutrient. These systems are solved by the Runge-Kutta method (Fig. 2–4); stationary modes are obtained, for which the values of the system parameters and initial conditions are determined.

The results obtained will be used for the further simulation of the phytoplankton dynamics considering the transformation of phosphorus, nitrogen and silica compounds, taking into account diffusion-convection, saltness, and temperature.

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